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M. Griebel

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Computer Science and Numerical Mathematics

M. Griebel

Institut für Angewandte Mathematik, Universität Bonn
Wegelerstr. 6, 53115 Bonn, Germany

The dramatic performance increase of computers in general, but especially of parallel supercomputers in recent years, opened up a new and exciting way to research in natural and engineering sciences: *numerical simulation*. Besides the traditional experimental and theoretical research approaches, a scientist may now use computers to gain insight into complex real world processes. To this end, a mathematical model based on experimental and observational data is developed. This model is then discretized with an appropriate numerical method and the resulting discrete problem must then be solved as efficiently as possible. Obviously the quality of the results is significantly dependent on the numerical method used and the quality of the discretization. In principle, this approach is applicable to a wide range of problems. But the resulting demands for storage and compute time on available computers is a limiting factor in practical applications. Hence, a major goal is the development of fast numerical methods with minimal storage requirements and their efficient implementation on large parallel computers. Another goal is to apply these techniques to practical problems from the natural and engineering sciences.

Most interesting problems can be modelled mathematically by systems of *partial differential equations*. Therefore, appropriate numerical discretization techniques such as finite elements, finite differences or finite volumes are of central interest. Here, the use of error estimators for the control of adaptive discretization techniques is a must to reduce the storage demands and to make three-dimensional problems with non-smooth solutions approachable. Furthermore, the fast and efficient numerical solution of the resulting large linear systems by multilevel and multigrid methods is important for efficiency reasons. Finally, all these components need to be combined and parallelized in a load-balanced fashion to be able to tackle real world problems.

These ingredients are the key to any successful and meaningful numerical simulation of three-dimensional problems. Consequently they are subject of intensive research. This is reflected in the following three articles which report on the results of numerical projects conducted on the Cray T3E in Jülich and other parallel supercomputers.

In the contribution *Hash based adaptive parallel multilevel methods with space filling curves* by M. Griebel and G. Zumbusch, the authors address the problem of load balancing. Especially for adaptively refined meshes, the optimal partitioning of data is in general a *NP*-hard problem. Therefore heuristics are needed. Here, a parallel and cheap method based on space-filling curves is used. The method is applied to elliptic boundary value problems. Its performance is demonstrated on two large parallel computers, namely the ASCI Blue Pacific and Jülich's Cray T3E.

The article *A parallel software-platform for solving problems of partial differential equations using unstructured grids and adaptive multigrid methods* by P. Bastian, K. Johannsen, S. Lang, S. Nägele, C. Wieners, V. Reichenberger, G. Wittum and C. Wrobel deals with the software aspects of complex simulation programs. The package UG is a

system to discretize and solve PDEs on unstructured grids. It uses finite element and finite volume techniques, features adaptive refinement and various parallel multigrid solvers, especially algebraic multigrid. Load balancing for parallelization is achieved by recursive coordinate bisection and similar partitioning techniques. Applications range from classical PDEs, over two-phase flows, elasticity and plasticity to the Navier-Stokes equations and turbulence modelling.

In the third contribution *High performance FEM simulation via FEAST and application to parallel CFD via FEATFLOW*, C. Becker, S. Buijssen, S. Kilian and S. Turek report on their efforts to simulate non-stationary laminar and turbulent flow problems in complex situations. Based on their FEAST and FEATFLOW program systems, the authors aim at a scalable recursive clustering approach. They discuss computational bottlenecks for parallel multigrid and domain decomposition, motivate the approach and show the results of their simulations for an industrial problem from steel casting.

Alltogether, these three numerical projects show how to efficiently bridge the gap between adaptive discretization techniques, multigrid solvers and parallel computing when it comes to practical three-dimensional simulations of real life problems on large supercomputers like the Cray T3E. It is on the basis of such techniques that numerical simulation already is and in the future even more will be a competitive and cost effective third way to gain further insight in the natural and engineering sciences.